

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF112019\
 Data File : BF117897.D
 Acq On : 20 Nov 2019 17:06
 Operator : JU
 Sample : K5927-06
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-5A

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.193	12	18	27	rVB	684870	917592	19.83%	2.427%
2	5.128	512	517	525	rVB	548536	667000	14.41%	1.764%
3	5.534	581	586	589	rBV	3324578	3123089	67.48%	8.261%
4	6.540	752	757	760	rBV	3478521	3328807	71.93%	8.806%
5	6.687	777	782	785	rBV	3902037	3537434	76.44%	9.358%
6	6.916	817	821	824	rBV	1264865	959251	20.73%	2.537%
7	7.075	844	848	851	rBV	3557097	2895410	62.56%	7.659%
8	7.481	912	917	920	rBV	2485049	2384311	51.52%	6.307%
9	8.204	1036	1040	1043	rBV	1663596	1353006	29.24%	3.579%
10	9.281	1219	1223	1226	rBV	5163603	4627993	100.00%	12.242%
11	9.363	1233	1237	1239	rBV	105719	93897	2.03%	0.248%
12	9.675	1286	1290	1295	rBV	852263	717150	15.50%	1.897%
13	9.892	1323	1327	1330	rVB	79078	72177	1.56%	0.191%
14	9.963	1336	1339	1343	rBV	1775091	1550070	33.49%	4.100%
15	10.392	1410	1412	1415	rVB	98912	70291	1.52%	0.186%
16	10.616	1446	1450	1456	rVB	64305	73996	1.60%	0.196%
17	10.757	1470	1474	1477	rBV	3051761	2576489	55.67%	6.816%
18	10.880	1490	1495	1499	rBV2	182238	240284	5.19%	0.636%
19	11.316	1566	1569	1572	rBV	98656	95624	2.07%	0.253%
20	11.351	1572	1575	1579	rVB	71260	76706	1.66%	0.203%
21	11.457	1589	1593	1597	rBV	1724859	1420294	30.69%	3.757%
22	11.522	1601	1604	1608	rVB2	75607	75943	1.64%	0.201%
23	11.745	1639	1642	1647	rVB	89482	77467	1.67%	0.205%
24	11.980	1678	1682	1686	rBV	397799	395375	8.54%	1.046%
25	12.157	1709	1712	1714	rBV	84730	73272	1.58%	0.194%
26	12.545	1775	1778	1784	rVB2	93701	96313	2.08%	0.255%
27	12.769	1812	1816	1820	rBV2	125224	144390	3.12%	0.382%
28	12.857	1828	1831	1836	rVB3	46124	56535	1.22%	0.150%
29	12.916	1838	1841	1845	rBV5	72136	88012	1.90%	0.233%
30	13.051	1859	1864	1867	rBV	3781742	3527954	76.23%	9.332%
31	13.492	1937	1939	1942	rBV2	49435	50282	1.09%	0.133%
32	13.951	2013	2017	2024	rBV	216088	348798	7.54%	0.923%
33	14.104	2040	2043	2047	rBV	1144410	1089632	23.54%	2.882%
34	15.621	2296	2301	2304	rBV	767398	998152	21.57%	2.640%

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ClientSampleId :
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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

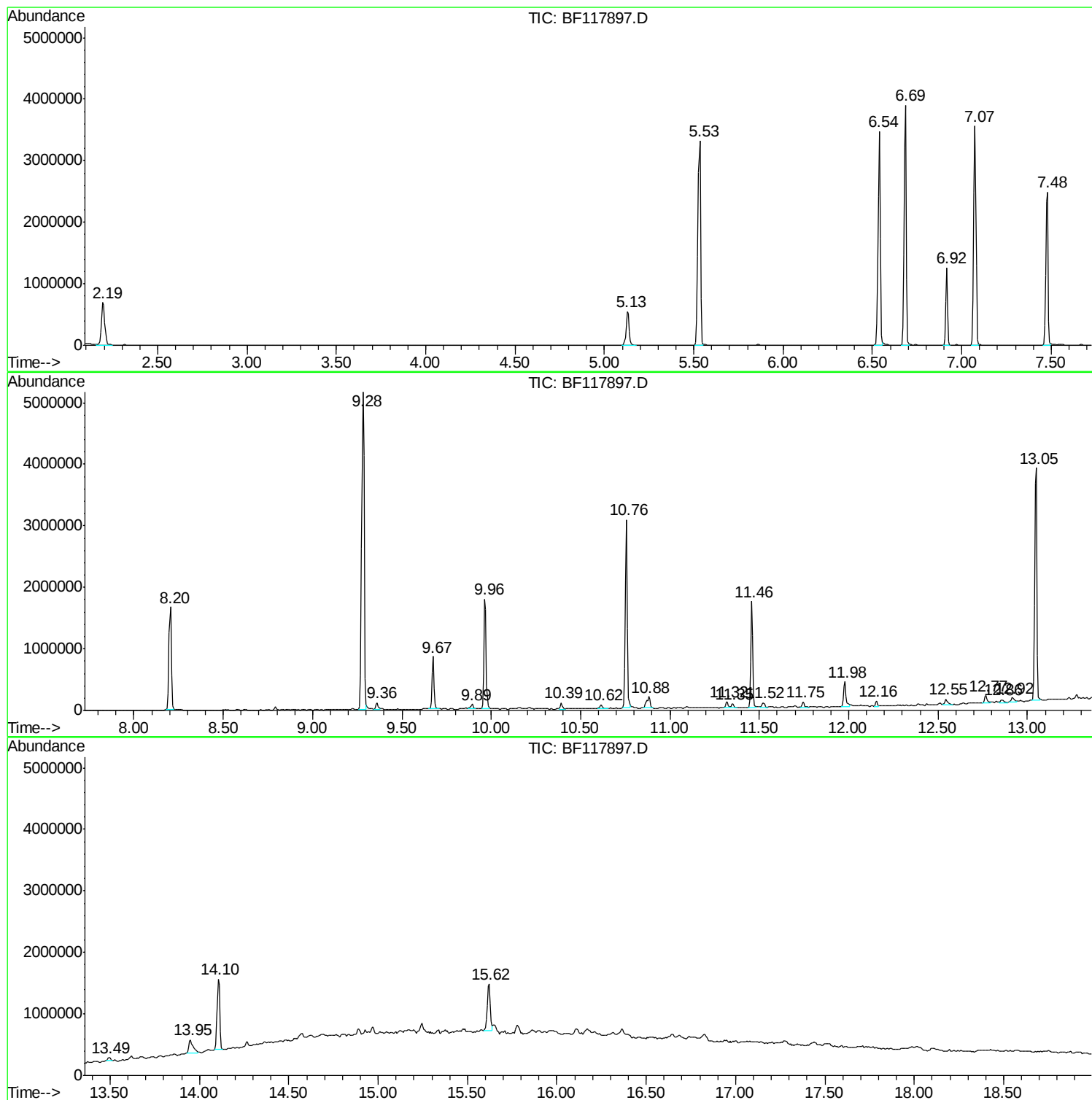
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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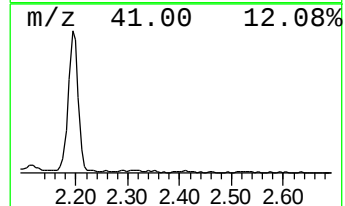
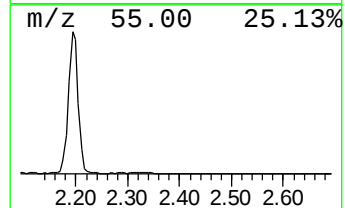
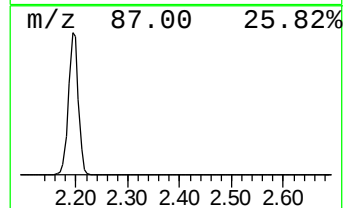
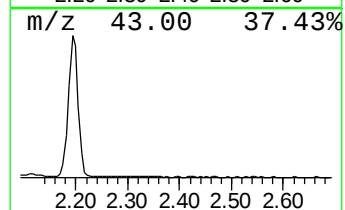
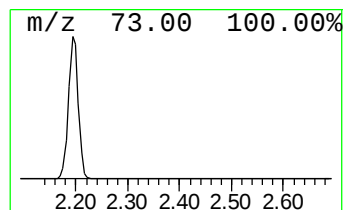
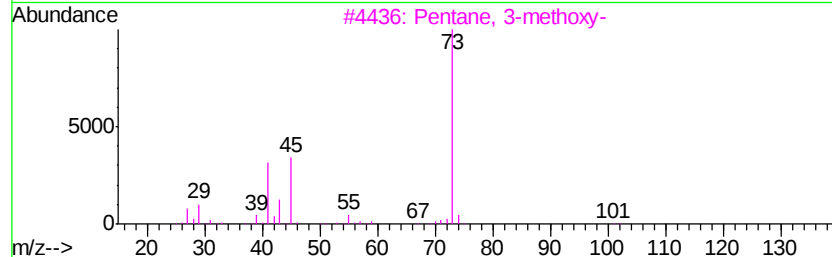
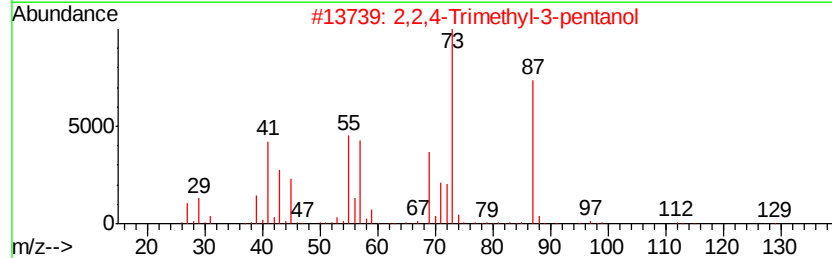
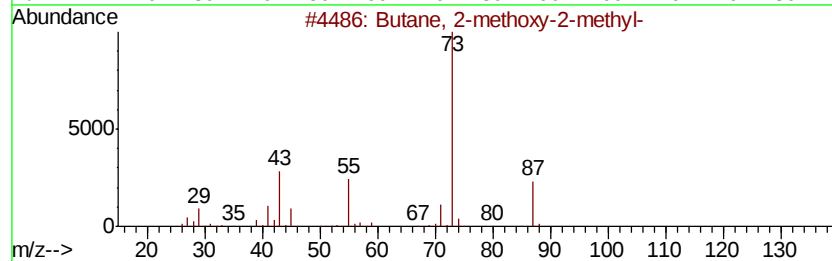
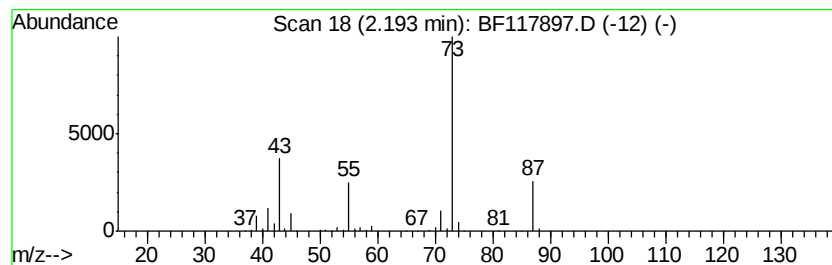
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.19	19.13 ng	917592	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4		N-Ethylformamide	73	C3H7NO	000627-45-2	9
5		Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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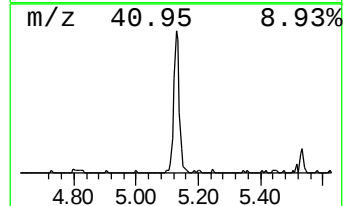
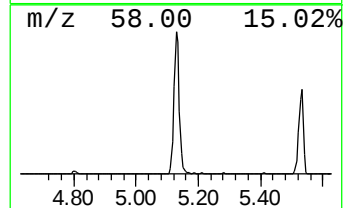
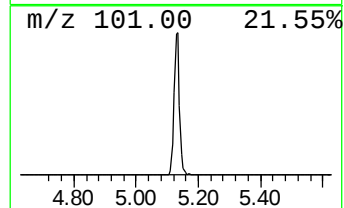
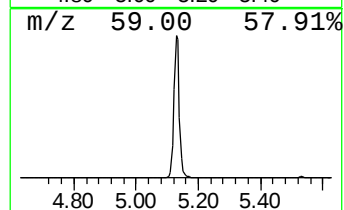
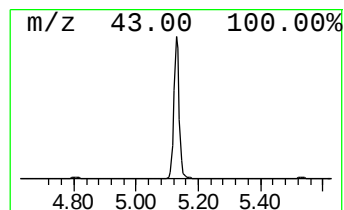
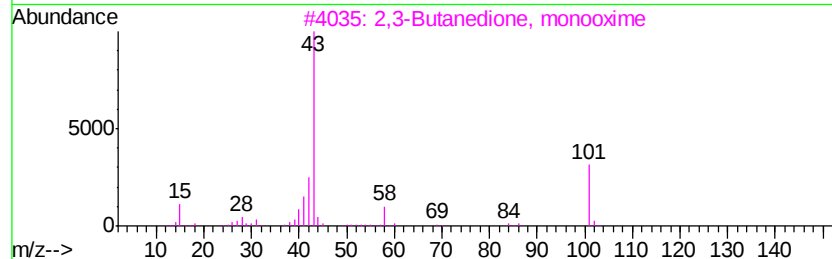
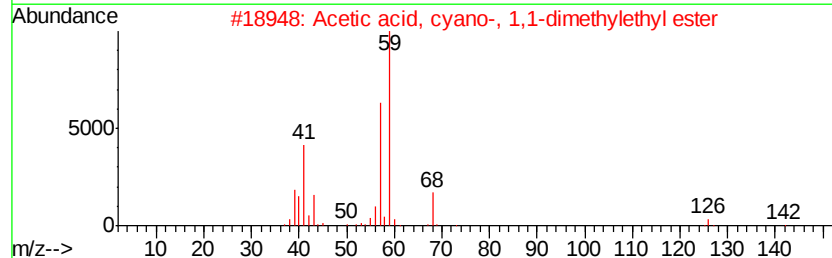
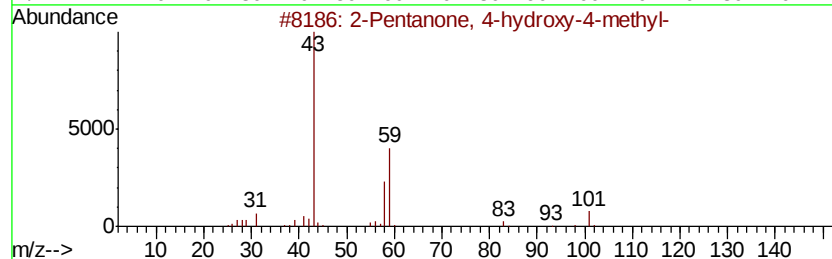
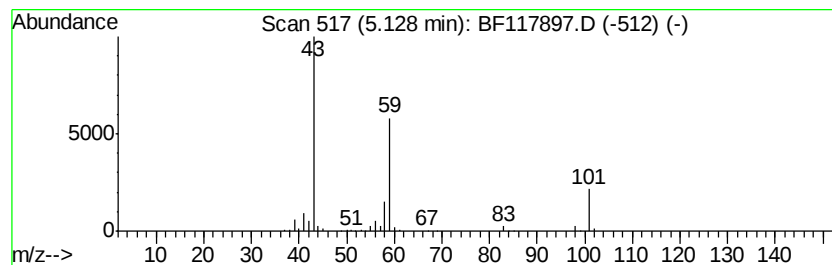
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown5.13 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	13.91 ng	667000	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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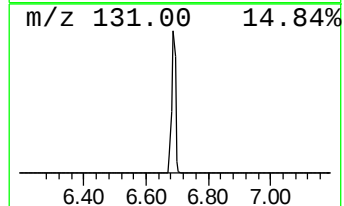
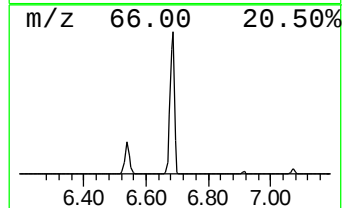
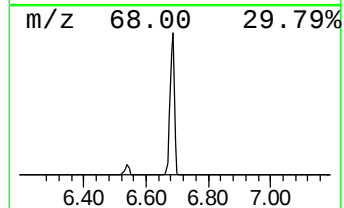
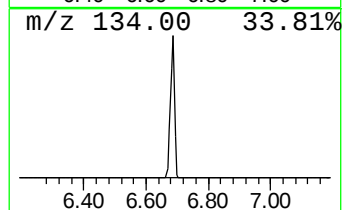
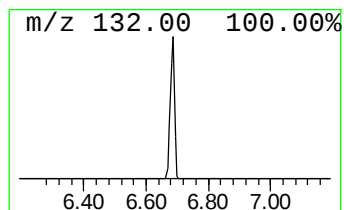
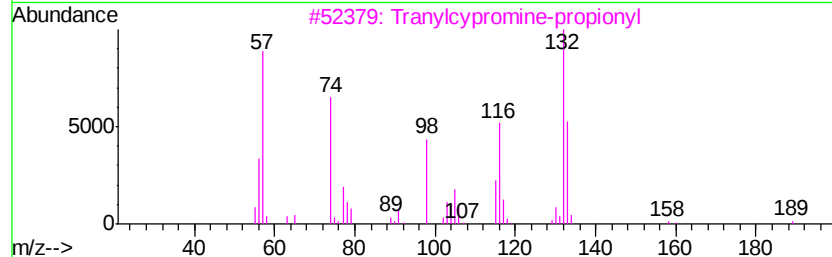
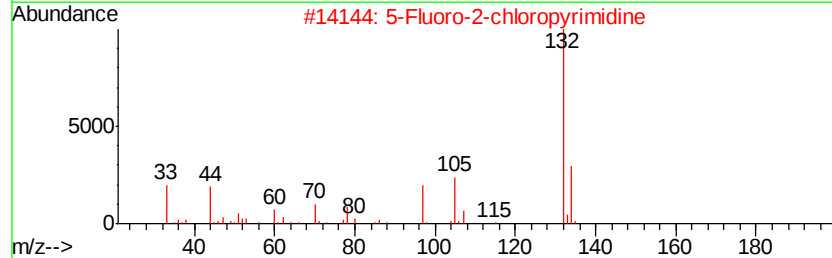
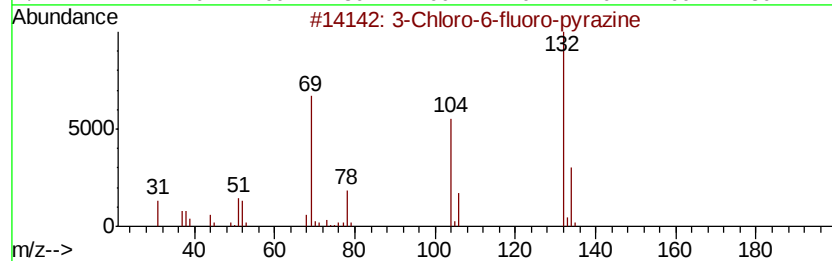
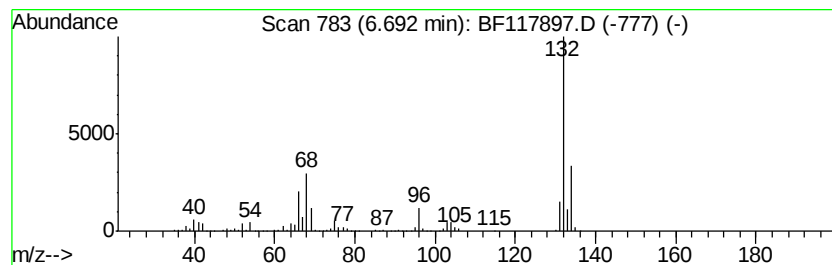
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	73.75 ng	3537430	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	25
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	16
4		5-Aminoindole	132	C8H8N2	005192-03-0	16
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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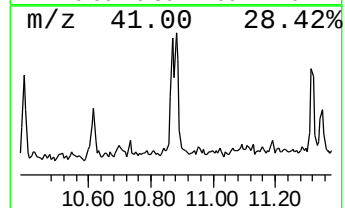
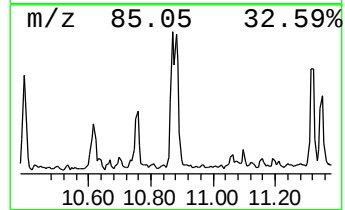
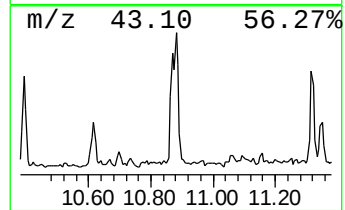
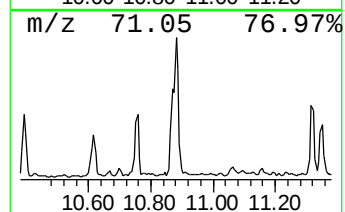
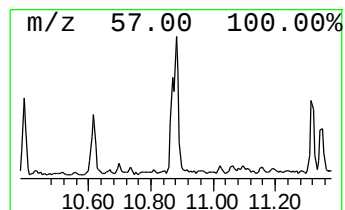
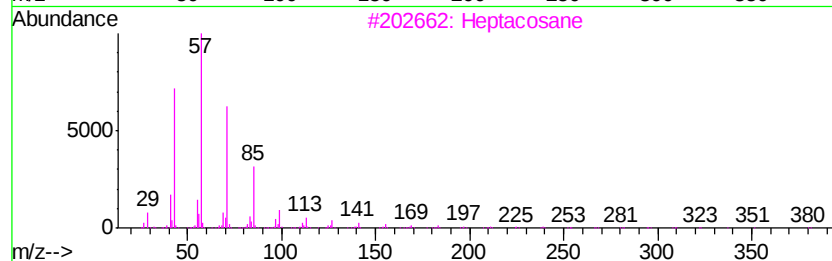
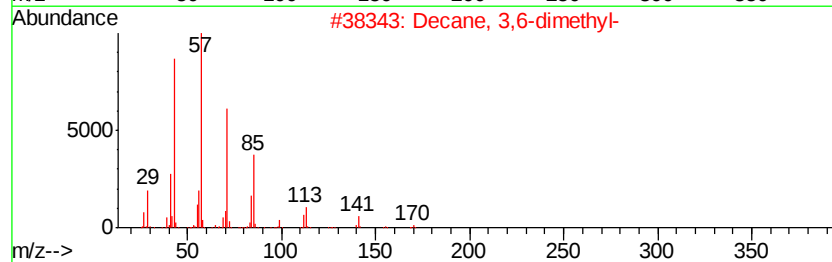
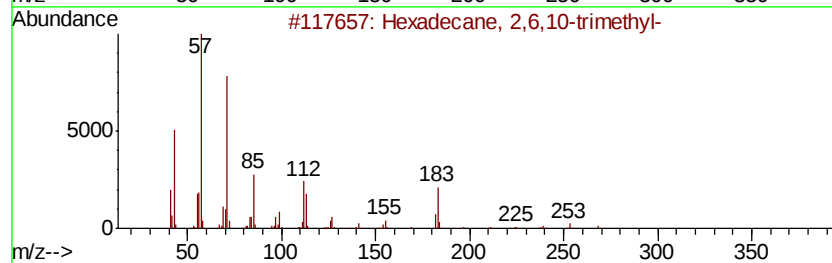
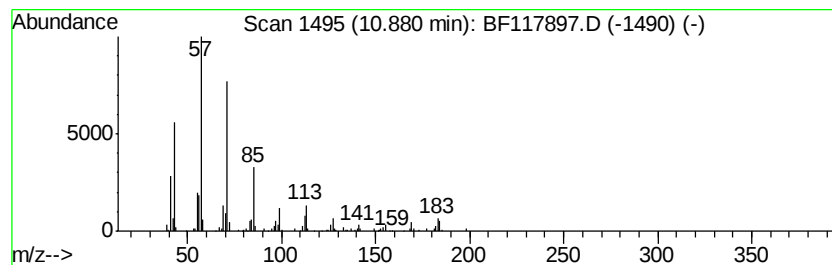
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TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 5 Hexadecane, 2,6,10-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.88	3.38 ng	240284	Phenanthrene-d10	11.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane, 2,6,10-trimethyl-	268	C19H40	055000-52-7	86
2		Decane, 3,6-dimethyl-	170	C12H26	017312-53-7	83
3		Heptacosane	380	C27H56	000593-49-7	80
4		Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	80
5		Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	80



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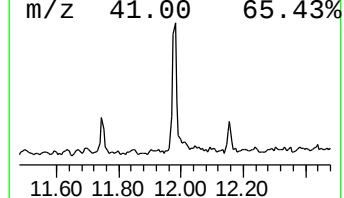
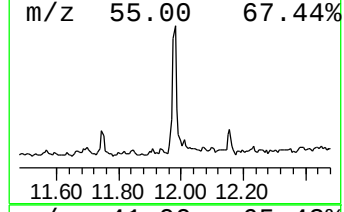
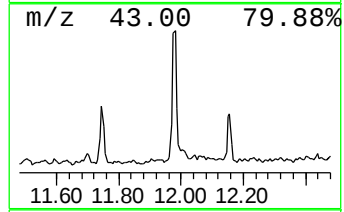
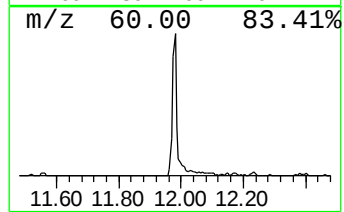
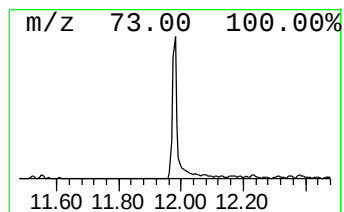
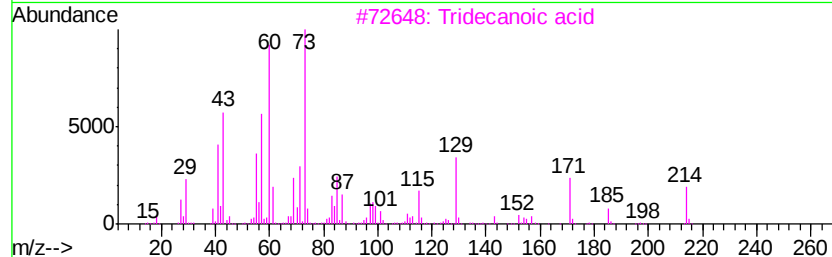
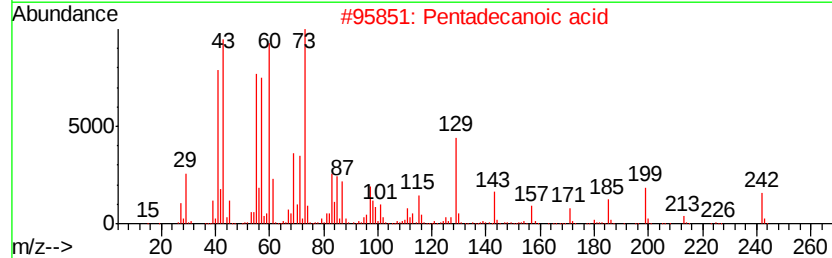
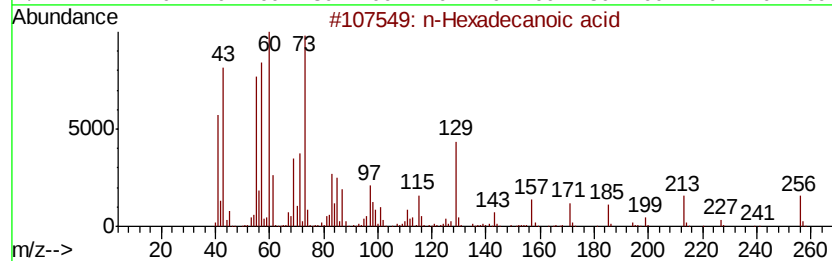
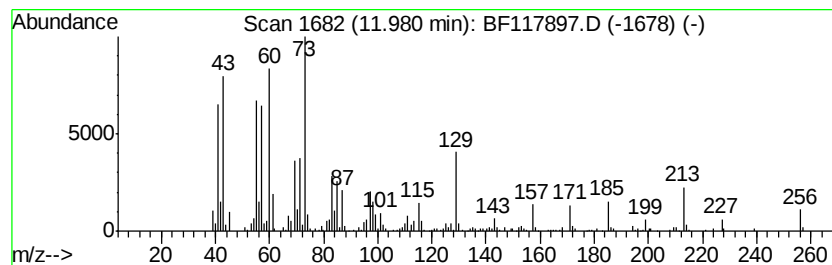
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.98	5.57 ng	395375	Phenanthrene-d10		11.46	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3		Tridecanoic acid	214	C13H26O2	000638-53-9	83
4		n-Decanoic acid	172	C10H20O2	000334-48-5	62
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	50



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ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-5A

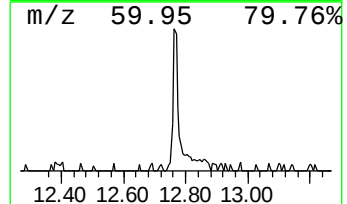
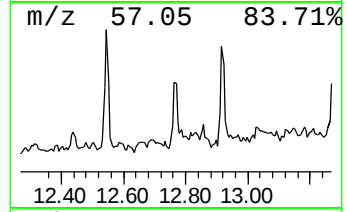
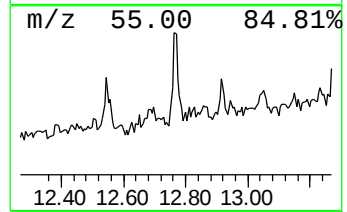
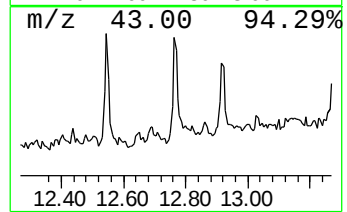
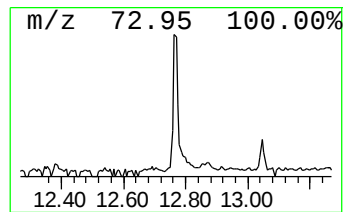
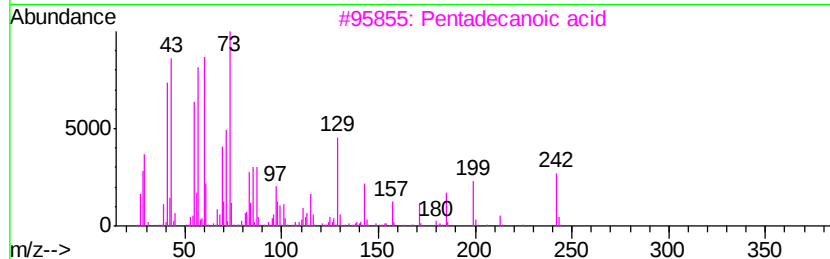
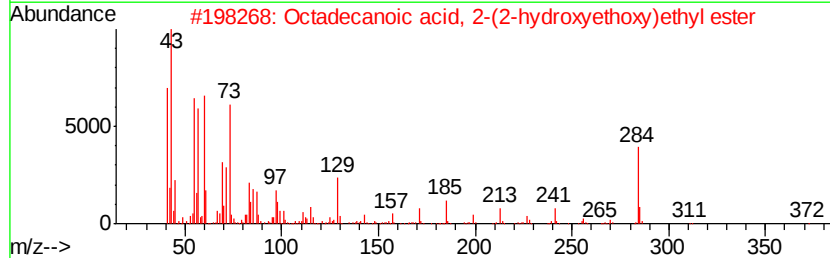
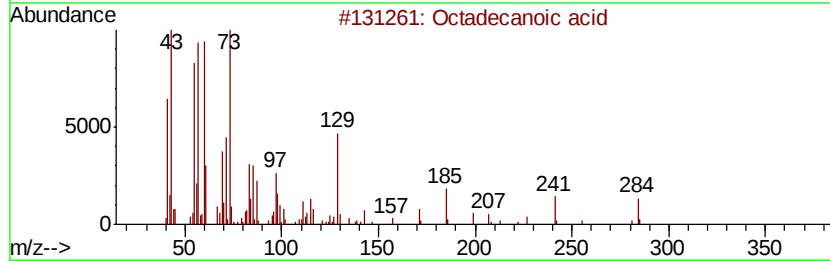
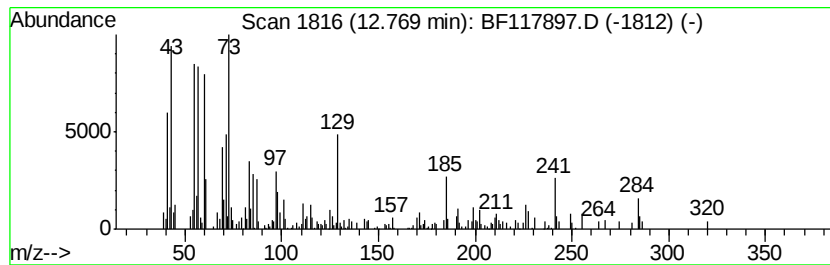
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.77	2.03 ng	144390	Phenanthrene-d10	11.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	90
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4		Tridecanoic acid	214	C13H26O2	000638-53-9	68
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112019\
Data File : BF117897.D
Acq On : 20 Nov 2019 17:06
Operator : JU
Sample : K5927-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-5A

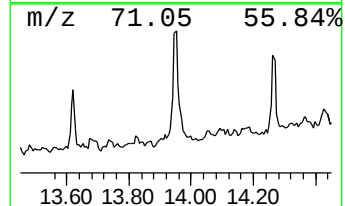
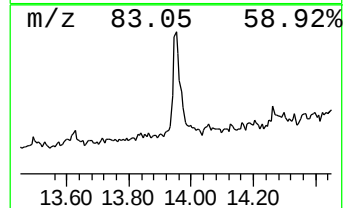
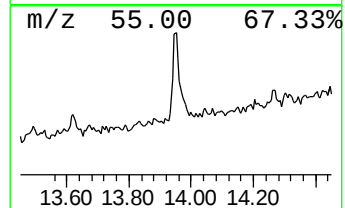
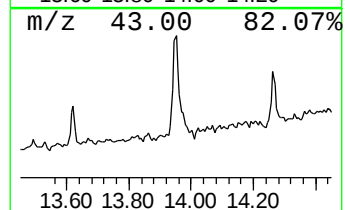
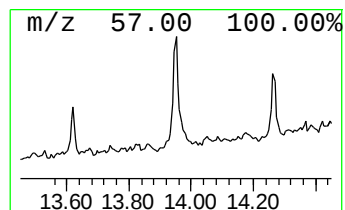
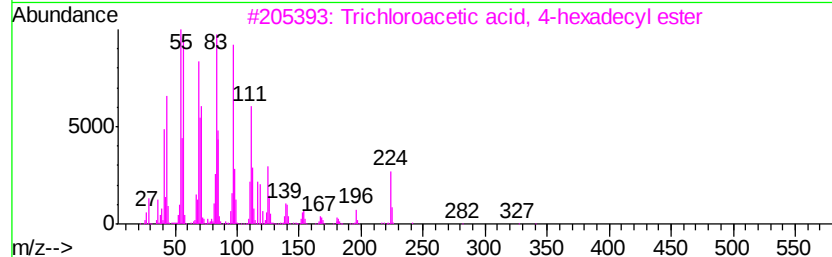
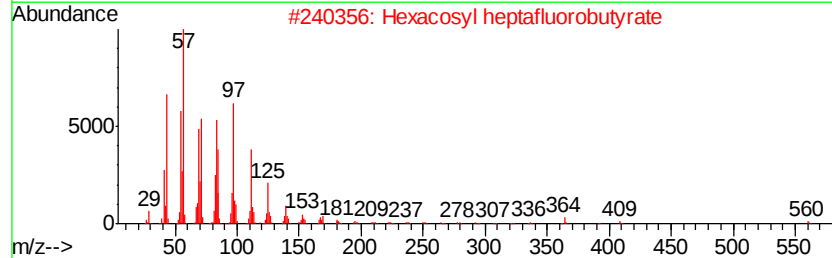
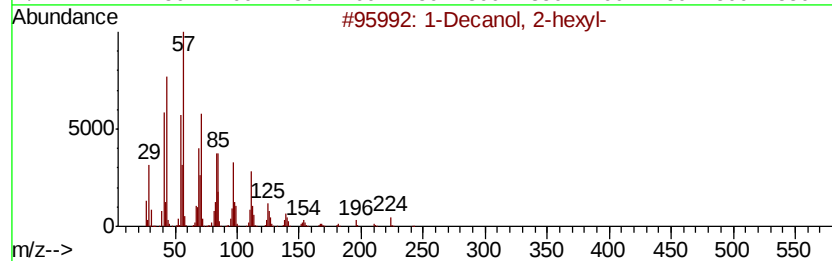
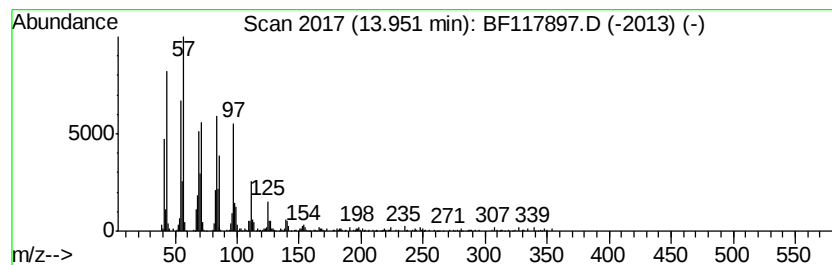
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 1-Decanol, 2-hexyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	6.40 ng	348798	Chrysene-d12	14.10

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	90
2		Hexacosyl heptafluorobutyrate	578	C30H53F7O2	1000351-83-3	86
3		Trichloroacetic acid, 4-hexadecyl...	386	C18H33Cl3O2	1000282-92-4	74
4		Hexacosyl trifluoroacetate	478	C28H53F3O2	1000351-75-0	74
5		Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	74



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF112019\
Data File : BF117897.D
Acq On : 20 Nov 2019 17:06
Operator : JU
Sample : K5927-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-5A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.19	19.1 ng		917592	1	6.92	959251	20.0
unknown5.13	5.13	13.9 ng		667000	1	6.92	959251	20.0
unknown6.69	6.69	73.8 ng		3537430	1	6.92	959251	20.0
Hexadecane, 2,6,1...	10.88	3.4 ng		240284	4	11.46	1420290	20.0
n-Hexadecanoic acid	11.98	5.6 ng		395375	4	11.46	1420290	20.0
Octadecanoic acid	12.77	2.0 ng		144390	4	11.46	1420290	20.0
1-Decanol, 2-hexyl-	13.95	6.4 ng		348798	5	14.10	1089630	20.0